Claims:

1. A method of designing a compound which binds to a molecule of the EGF receptor family and modulates an activity mediated by the molecule, which method comprises the step of assessing the stereochemical complementarity between the compound and a topographic region of the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

2. A method as claimed in claim 1 in which the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

3. A method as claimed in claim 1 in which the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

4. A method as claimed in any one of claims 1 to 3 in which the compound is designed so as to complement the structure of a topographic region of the molecule as depicted in Figure 5.

5. A method as claimed in any one of claims 1 to 4, in which the compound has structural regions able to make close contact with amino acid residues at the surface of the molecule lining the groove as depicted in Figure 7, Figure 8 or Figure 9.

6. A method as claimed in any one of claims 1 to 5, in which the compound has a stereochemistry such that it can interact with both the L1 and L2 domains of the molecule.

7. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the region of the L1 domain-S1 domain interface, causing an alteration in the positions of the L1 and S1 domains relative to each other.

8. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the hinge region between the L2 domain and the S1 domain causing an alteration in the positions of the L2 and S1 domains relative to each other.

9. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the β-sheet of the L1 domain causing an alteration in the position of the L1 domain relative to the position of the S1 domain or the L2 domain.

10. A method as claimed in any one of claims 1 to 5 in which the compound has a stereochemistry such that it can interact with both the L2 and S2 domains of the molecule.

11. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the hinge region between the L2 domain and the S2 domains causing an alteration in the positions of the L1 and L2 domains relative to each other.

12. A method as claimed in any one of claims 1 to 5, in which the compound interacts with the β-sheet of the L2 domain causing an alteration in the position of the L2 domain relative to the position of the S2 domain.

13. A method as claimed in any one of claims 1 to 5, in which the compound binds to a lower face containing the second β-sheet of the L1 and/or L2 domains, wherein the structure of the face is characterised by a plurality of solvent-exposed hydrophobic residues.

14. A method according to claim 13, in which the hydrophobic residues include:

(i) Tyr64, Leu66, Tyr89, Tyr93; and/or

(ii) Leu348, Phe380 and Phe412.

15. A method as claimed in anyone of claims 1 to 14, in which the stereochemical complementarity between the compound and the receptor site is such that the compound has a K_d for the receptor site of less than 10^{-6}M.

16. A method as claimed in claim 15 in which the K_d is less than 10^{-8}M.

17. A method as claimed in any one of claims 1 to 16 in which the compound is selected or modified from a known compound identified from a data base.

18. A method according to any one of claims 1 to 17, in which the compound has the ability to increase an activity mediated by a molecule of the EGF receptor family.

19. A method according to any one of claims 1 to 18, in which the compound has the ability to decrease an activity mediated by a molecule of the EGF receptor family.

20. A method according to claim 19, in which the stereochemical interaction between the compound and the molecule is adapted to prevent the binding of a natural ligand of the receptor molecule to the receptor site.

21. A method according to claim 19 or claim 20, in which the compound has a K_i of less than 10^{-6}M.

22. A method according to claim 21, in which the compound has a K_I of less than 10^{-6}M.

23. A method according to claim 22, in which the compound has a K_I of less than 10^{-9}M.

24. A computer-assisted method for identifying potential compounds able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, using a programmed computer comprising a processor, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer, through the input device, data comprising the atomic coordinates of the EGF receptor molecule as shown in Figure 6, or a subset thereof;

(b) generating, using computer methods, a set of atomic coordinates of a structure that possesses stereochemical complementarity to the atomic coordinates of a topographic region of the EGF receptor molecule as shown in Figure 6, or a subset thereof, thereby generating a criteria data set;

(c) comparing, using the processor, the criteria data set to a computer database of chemical structures;

(d) selecting from the database, using computer methods, chemical structures which are similar to at least a portion of said criteria data set; and

(e) outputting, to the output device, the selected chemical structures which are similar to a portion of the criteria data set.

25. A computer-assisted method according to claim 24, in which the method is used to identify potential compounds which have the ability to decrease an activity mediated by the molecule.

26. A computer-assisted method according to claim 24 ~~or claim 25~~, which further comprises the step of selecting one or more chemical structures from step (e) which interact with the molecule in a manner which prevents the binding of natural ligands to the molecule.

27. A computer-assisted method according to ~~any one of~~ claims 24 ~~to 26~~, which further comprises the step of obtaining a compound with a chemical

structure selected in steps (d) and (e), and testing the compound for the ability to decrease an activity mediated by the molecule.

28. A computer-assisted method according to claim 24, in which the method is used to identify potential compounds which have the ability to increase an activity mediated by the molecule.

29. A computer-assisted method according to claim 28, further comprising the step of obtaining a compound with a chemical structure selected in steps (d) and (e), and testing the compound for the ability to increase an activity mediated by the receptor.

30. A method of screening a putative compound having the ability to modulate the activity of a molecule of the EGF receptor family, comprising the steps of identifying a putative compound by a method according to any one of claims 1 to 29, and testing the compound for the ability to increase or decrease an activity mediated by the molecule.

31. A method according to claim 30, in which the test is carried out *in vitro*.

32. A method according to claim 31, in which the test is a high throughput assay.

33. A method according to claim 30, in which the test is carried out *in vivo*.

34. A method as claimed in ~~any one of~~ claims 1 ~~to 33~~ in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

35. A method as claimed in claim 34 in which the molecule of the EGF receptor family is the EGF receptor.

36. A compound able to bind to a molecule of the EGF receptor family and to modulate an activity mediated by the molecule, the compound being obtained by a method according to ~~any one of~~ claims 1 ~~to 35~~.

37. A compound which possesses stereochemical complementarity to a topographic region of a molecule of the EGF receptor family and modulates an activity mediated by the molecule, wherein the molecule is characterised by

(i) amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

(ii) one or more subsets of said amino acids related to the coordinates shown in Figure 6 by whole body translations and/or rotations; or

(iii) amino acids present in the amino acid sequence of a member of the EGF receptor family, which form an equivalent three-dimensional structure to that of the receptor site defined by amino acids 1-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6;

with the proviso that the compound is not a naturally occurring ligand of a molecule of the EGF receptor family or a mutant thereof.

38. A compound as claimed in claim 37 in which the topographic region of the molecule is defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 1-475 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

39. A compound as claimed in claim 37 in which the topographic region of the molecule is defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6, or an amino acid sequence which forms an equivalent three-dimensional structure to that of the region defined by amino acids 313-621 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6.

40. A compound as claimed in ~~anyone of~~ claims 37 ~~to 39,~~ in which the stereochemical complementarity between the compound and the molecule is such that the compound has a K_d for the receptor site of less than 10^{-6}M.

41. A compound as claimed in claim 40 in which the K_d is less than 10^{-8}M.

42. A compound as claimed in ~~any one of~~ claims 36 ~~to 41~~, wherein the compound increases an activity mediated by a molecule of the EGF receptor family.

43. A compound as claimed in ~~any one of~~ claims 36 ~~to 41~~, wherein the compound decreases an activity mediated by a molecule of the EGF receptor family.

44. A compound as claimed in ~~any one of~~ claims 36 ~~to 43~~ in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

45. A compound as claimed in claim 44 in which the molecule of the EGF receptor family is the EGF receptor.

46. A pharmaceutical composition for preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family, which comprises a compound as claimed in claim 42 and a pharmaceutically acceptable carrier or diluent.

47. A pharmaceutical composition for preventing or treating a disease associated with signalling by a molecule of the EGF receptor family, which comprises a compound as claimed in claim 43 and a pharmaceutically acceptable carrier or diluent.

48. A method of preventing or treating a disease which would benefit from increased signalling by a molecule of the EGF receptor family which method comprises administering to a subject in need thereof a compound as claimed in claim 42.

49. A method according to claim 48 wherein the disease is selected from wound healing and gastric ulcers.

50. A method of preventing or treating a disease associated with signalling by a molecule of the EGF receptor family which method comprises

administering to a subject in need thereof a compound as claimed in claim 43.

51. A method according to claim 50 wherein the disease is selected from psoriasis and tumour states consisting of cancer of the breast, brain, ovary, cervix, pancreas, lung, head and neck, and melanoma, rhabdomyosarcoma, mesothelioma and glioblastoma.

52. A method as claimed in ~~any one of~~ claims 48 ~~to 51~~ in which the molecule of the EGF receptor family is selected from the group consisting of the EGF receptor, ErbB2, ErbB3 and ErbB4.

53. A method as claimed in claim 52 in which the molecule of the EGF receptor family is the EGF receptor.